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**Manipulating Two-Dimensional Semiconducting Materials for
Nanoelectronics and Energy Conversion**

By

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Abstract

Two-dimensional (2D) semiconducting materials, such as phosphorene,

MoS₂, et al. hold great promise for many important applications, such as in nanoelectronics, molecular and bio-sensors, thermoelectric conversion and solar energy harvesting. To fully explore their functionalities and potentials, band-gap engineering is often required. It is now recognized that these 2D materials are able to subject to strain, chemical functionalization, size reduction, which can cause significant changes in electronic, optical, magnetic and thermal properties, which in turn can greatly widen the range of applications of 2D materials. In this talk, we report our research work on the manipulation of two members of 2D semiconducting materials, that is, phosphorene and MoS₂, to tune their electronic, magnetic and thermal properties using first-principles calculations. Our work demonstrates various practical routes to tune the electronic properties of 2D semiconducting materials by strain engineering, chemical functionalization and size manipulation, which may be useful for applications in nanoelectronic devices and energy conversion.

Biography

Dr. ZHANG Yong-Wei is Principal Scientist and Deputy Executive Director at Institute of High Performance Computing (IHPC), A*STAR, Singapore. He received Ph.D from Northwestern Polytechnical University, China. Subsequently he worked at Institute of Mechanics, Chinese Academy of Sciences, China; Division of Engineering at Brown University, USA; Institute of Materials Research and Engineering, A*STAR, Singapore; and Department of Materials science and Engineering at National University of Singapore. His interests focus on using theory, modeling and computation as tools to study the relationship between structures and properties of materials with applications in material design, property engineering, mechanical-thermal coupling and mechanical-electronic coupling *et al.* He has published over 280 refereed journal papers, and delivered over 50 invited talks and lectures. He is a winner of the High Performance Computing Quest Gold Award (2004), IHPC Best Paper Award (2011, 2012, 2013), IHPC Best Industry Project Award (2013), and A*Star Aerospace Programme Achievement Award (2013).

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